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APS Upgrade: Connecting Proteins to Organisms

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One of the grand challenges in the life sciences is to connect our understanding of proteins on the structural level to their function within organisms through their role in organelles, cells, organs, and beyond. Other important molecules of life such as RNA and DNA are involved in replication, carbohydrates in recognition, membrane proteins in signaling and transport, and macromolecular complexes and assemblies in cellular function. Crystallography is an essential tool towards the goal of understanding the structure of the individual components and their complexes. In addition to improving throughput, it will be necessary to enable techniques that can circumvent existing bottlenecks such as the difficulty in obtaining adequate crystals. For example, microcrystallography promises to allow data collection from micron-sized crystals as well as reducing the radiation damage to an exposed micron-sized area. Beyond determining static crystal structures, it is vital to further our understanding of protein dynamics and conformational changes. This is achievable through inelastic scattering as well as through direct ultrafast scattering and spectroscopy. The behavior of proteins in conditions typical of *in vivo* systems (e.g., in solution), protein folding, protein-protein interactions, and drug/ligand binding can be studied using small-angle and wide-angle x-ray scattering (SAXS/WAXS) techniques. Connecting to proteins' function in organisms, in particular under environmental factors such as the local chemical/trace elemental environment, can be addressed by using tools such as the cryo-nanoprobe beamline. This will allow the visualization of trace elemental content in biological systems down to the level of 10's of nanometers, detecting as few as 10 metal atoms for specific elements in ideal samples. Not only will this further our fundamental understanding of biological systems and their interaction with the local environment but also have significant impact on applications in health and disease as well as environmental stewardship. Ancillary equipment will facilitate correlative experiments as well as allow supplemental studies (e.g., optimum freezing/vitrification techniques).

We will give an overview of projects planned with regards to the proposed APS upgrade, with emphasis on (1) cryo-nanoprobe beamline, (2) enhanced SAXS/WAXS beamline, (3) microfocus macromolecular crystallography (MX) beamline, (4) enhanced time-resolved MX beamline, and (5) cryo sample prep/analysis facility.